

# Kamal Sharkas

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5654835/publications.pdf>

Version: 2024-02-01

19  
papers

820  
citations

516710

16  
h-index

794594

19  
g-index

19  
all docs

19  
docs citations

19  
times ranked

804  
citing authors

#	ARTICLE	IF	CITATIONS
1	Fermi-Löwdin orbital self-interaction correction of adsorption energies on transition metal ions. <i>Journal of Chemical Physics</i> , 2022, 156, 134102.	3.0	2
2	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18678-18685.	2.8	14
3	Self-interaction error overbinds water clusters but cancels in structural energy differences. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 11283-11288.	7.1	57
4	Towards efficient density functional theory calculations without self-interaction: The Fermi-Löwdin orbital self-interaction correction. <i>Journal of Physics: Conference Series</i> , 2019, 1290, 012002.	0.4	17
5	The effect of self-interaction error on electrostatic dipoles calculated using density functional theory. <i>Journal of Chemical Physics</i> , 2019, 151, 174106.	3.0	29
6	The effects of active site and support on hydrogen elimination over transition-metal-functionalized yttria-decorated metal-organic frameworks. <i>Catalysis Science and Technology</i> , 2019, 9, 7003-7015.	4.1	5
7	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 126-138.	5.3	40
8	Shrinking Self-Interaction Errors with the Fermi-Löwdin Orbital Self-Interaction-Corrected Density Functional Approximation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9307-9315.	2.5	30
9	Fermi-Löwdin orbital self-interaction correction to magnetic exchange couplings. <i>Journal of Chemical Physics</i> , 2018, 149, 164101.	3.0	33
10	Multiconfiguration Pair-Density Functional Theory and Complete Active Space Second Order Perturbation Theory. Bond Dissociation Energies of FeC, NiC, FeS, NiS, FeSe, and NiSe. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9392-9400.	2.5	27
11	Range-separated double-hybrid density-functional theory applied to periodic systems. <i>Journal of Chemical Physics</i> , 2015, 143, 102811.	3.0	21
12	Calculating NMR Chemical Shifts for Paramagnetic Metal Complexes from First-Principles. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2183-2188.	4.6	64
13	Effects from Spin-Orbit Coupling on Electron-Nucleus Hyperfine Coupling Calculated at the Restricted Active Space Level for Kramers Doublets. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 538-549.	5.3	32
14	Double-hybrid density-functional theory applied to molecular crystals. <i>Journal of Chemical Physics</i> , 2014, 141, 044105.	3.0	24
15	Double-hybrid density-functional theory with meta-generalized-gradient approximations. <i>Journal of Chemical Physics</i> , 2014, 140, 084107.	3.0	35
16	A multiconfigurational hybrid density-functional theory. <i>Journal of Chemical Physics</i> , 2012, 137, 044104.	3.0	77
17	Double-hybrid density-functional theory made rigorous. <i>Journal of Chemical Physics</i> , 2011, 134, 064113.	3.0	165
18	Communication: Rationale for a new class of double-hybrid approximations in density-functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 101102.	3.0	93

#	ARTICLE	IF	CITATIONS
19	Ab initio study of the chemical states of water on Cr <sub>2</sub> O <sub>3</sub> (0001): From the isolated molecule to saturation coverage. Surface Science, 2009, 603, 2484-2493.	1.9	55